imaginary time: for a finite grid the error in estimating derivatives $G^{(m)}$ increases rapidly with order m; thus, the determination of high order moments $\langle(\omega-\mu)^m\rangle_{A(\omega)}$ of the spectrum is in general an ill-posed problem. At low temperatures, $G(\beta/2)$ gives a hint as to the weight of a quasiparticle peak or the existence of a gap via (1.60) since its value is proportional to the value of the spectral function near the Fermi energy, averaged over an inverse hyperbolic cosine with width π/β.

First attempts to address the analytic continuation problem for QMC data included least-squares fits, Padé approximants, and regularization (for references, see the pedagogical and concise review by Jarrell (1997)). Least-squares fits of spectra approximated as a set of box functions are inherently unstable. Padé approximations for $G(i\omega_n)$ only work well for very precise data (e.g., in the context of Eliashberg equations), but not for QMC. Regularization of the kernel (1.56) tends to produce overly smeared-out spectra. What is needed instead is a regularization of the solution $A(\omega)$ that only shows features which are supported by the data, but is as smooth as possible otherwise. This is essentially the idea of the maximum entropy method (MEM) of finding the most probable spectrum compatible with the data.

The MEM is a very general approach for reconstructing continuous, positive semidefinite functions (i.e., densities or spectra) from incomplete, noisy, and possibly oversampled[28] data. It has a long history in the context of image reconstruction in such diverse disciplines as radio aperture synthesis, optical deconvolution, X-ray imaging, structural molecular biology, and medical tomography (see Skilling and Bryan (1984) and references therein). A preliminary study of its usefulness in the context of the analytic continuation problem (Silver, Sivia, and Gubernatis, 1990) was soon followed by applications to spectra (Silver, Gubernatis, Sivia, and Jarrell, 1990; Jarrell, Sivia, and Patton, 1990) and correlation functions (Deisz, Jarrell, and Cox, 1990). An efficient and general formulation of a MEM algorithm for analytic continuation of (oversampled) QMC data was then given by Gubernatis, Jarrell, Silver, and Sivia (1991), closely following the general state-of-the-art approach by Bryan (1990).

For simplicity, we will first assume that the QMC simulation produces N_d measurements of the observables $G_l \equiv G(l\Delta\tau)$, $0 \le l < \Lambda$ which are independent both in computer time and in imaginary time, i.e., without significant autocorrelation between subsequent measurements or between adjacent imaginary time slices.[29] If we further disregard systematic errors and assume some "true" spectrum A [which corresponds to a discretized Green function G_l via (1.55)] as well as a Gaussian distribution of statistical errors, the probability distribution for the observed averaged

[28]Data is called *oversampled* when measurements of different data points (here: for different τ) are not statistically independent, but correlated (Bryan, 1990). In this case, the number of "good" degrees of freedom (entering the error statistics) is reduced.

[29]Typically, one of the "measurements" of a set $\{G_l\}$ is generated by binning a macroscopic number of measurements within QMC. Autocorrelation in computer time, i.e., between different bins vanishes in the limit of infinite bin size.